

structures within a given mineral suggests that the isotopic signatures of soil (oxy) hydroxide could be heterogeneous.

Density functional and correlated molecular orbital calculations (MP2) are carried out on $B(OH)_3 \cdot nH_2O$ clusters ($n = 0, 6, 32$) and $B(OH)_4 \cdot nH_2O$ ($n = 0, 8, 11, 32$) to estimate the equilibrium distribution of ^{10}B and ^{11}B isotopes between boric acid and borate in aqueous solution. For the large 32-water clusters, multiple conformations are generated from ab initio molecular dynamics simulations to account for the effect of solvent fluctuations on

the isotopic fractionation. We provide an extrapolated value of the equilibrium constant \hat{a}_{34} for the isotope exchange reaction $^{10}B(OH)_3(aq) + ^{11}B(OH)_4(aq) = ^{11}B(OH)_3(aq) + ^{10}B(OH)_4(aq)$ of 1.026—1.028 near the MP2 complete basis set limit with 32 explicit waters of solvation. With some exchange-correlation functionals we find potentially important contributions from a tetrahedral neutral $B(OH)_3 \cdot H_2O$ Lewis acid–base complex. The extrapolations presented here suggest that DFT calculations give a value for $103 \ln \hat{a}_{34}$ about 15 % higher than the MP2 calculations.

Interaction of earthquakes and slow slip: Insights from fault models governed by lab-derived friction laws

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Motion of plates in the Earth crust is accommodated through fault slip. That includes both fast events (earthquakes) and slow relative motion, as evidenced by seismic and geodetic observations. We study mechanics and physics of earthquakes using a unique simulation approach that reproduces both earthquakes and slow slip, with full inclusion of inertial effects during simulated earthquakes, in the context of a 3D fault model. The approach incorporates laboratory-derived rate and state friction laws, including the effects of

shear heating during rapid, seismic slip, involves slow, tectonic-like loading, resolves all stages of seismic and aseismic slip, and results in realistic rupture speeds, slip velocities, and stress drops. Our simulations show that a number of observed earthquake phenomena can be explained by interaction of earthquakes and slow slip, including transition to intersonic rupture speeds during earthquakes, peculiar properties of small repeating earthquakes, and complex spatio-temporal patterns of earthquake sequences.

Numerical simulations of short-timescale geomagnetic field variations

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Numerical modeling of the convection in the Earth's liquid outer core has succeeded in simulating generation of a dipole-dominated magnetic field and its intermittent polarity reversals. However, previous models have used unrealistically high viscos-

ity for the core fluid because of computational difficulty to resolve small-scale turbulence that would otherwise happen. It is still an open question whether lower-viscosity Earth-type dynamo models can simulate the geomagnetic field and its time varia-

tions. Recent models have succeeded in reducing viscosity by about one order of magnitude, compared to previous models. However, such models seem to fail to produce an Earth-like strong magnetic field even though the viscosity is more realistic. I explained that this paradoxical result was caused by geophysically unrealistic boundary condition for the core surface temperature (Sakuraba, Roberts, *Nature Geosci.* **2009**. — **2**. 802 p.). If the core surface temperature is laterally uniform like recent low-viscosity models, the magnetic field is dipolar but its strength is relatively weak. If the surface heat flux is laterally uniform, which allows a pole-equator temperature difference, westward (retrograde) thermal wind naturally blows beneath the core equator and generates a strong toroidal magnetic field by its omega effect. The resultant dipole moment is relatively strong too. I concluded that the former boundary condition was not only theoretically unrealistic at the Earth's core-mantle boundary, but failed to produce Earth-like magnetic fields.

Small viscosity generally enables the dynamo model to simulate field variations of short timescales. Here I report on attempts to find Earth-like signa-

tures of short-timescale field variations in the low-viscosity geodynamo model. I focus on three characteristic geomagnetic secular variations: westward drift, torsional oscillations, and jerks. The simulated westward drift is confined in the equatorial belt like the geomagnetic field variations for the last 400 years. The drift is primarily caused by advection, but larger-scale (lower-wavenumber) fields tend to be stationary or rather move eastward, which suggests that some planetary-scale MHD waves modulate the field behaviors. The drift velocity is slower than the Earth's probably because the simulated magnetic Reynolds number is too small. The axial angular velocity of a cylinder in the liquid outer core can be defined as a function of the cylinder's radius and the time, and this shows wavelike propagation both toward the rotation axis and toward the core equator. The phase velocity is slightly slower than that predicted by the Braginsky's theory of torsional oscillations. All three magnetic field components in my model sometimes show zigzag variations in time like the geomagnetic jerk. The simulated jerk seems to be a local phenomenon, but the cause is still under investigation.